L-Proline, N-(2,5-ditrifluoromethylbenzoyl)-, undecyl ester

Inchi: InChI=1S/C25H33F6NO3/c1-2-3-4-5-6-7-8-9-10-16-35-23(34)21-12-11-15-32(21)22(33)1

InchiKey: UHMYESDHTSDVQV-UHFFFAOYSA-N

Formula: C25H33F6NO3

SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 509.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.55		Crippen Method
logp	7.403		Crippen Method
mcvol	358.100	ml/mol	McGowan Method
rinpol	2647.00		NIST Webbook
rinpol	2647.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U345983&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.